PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Overcoming Barriers for Dilute Combustion

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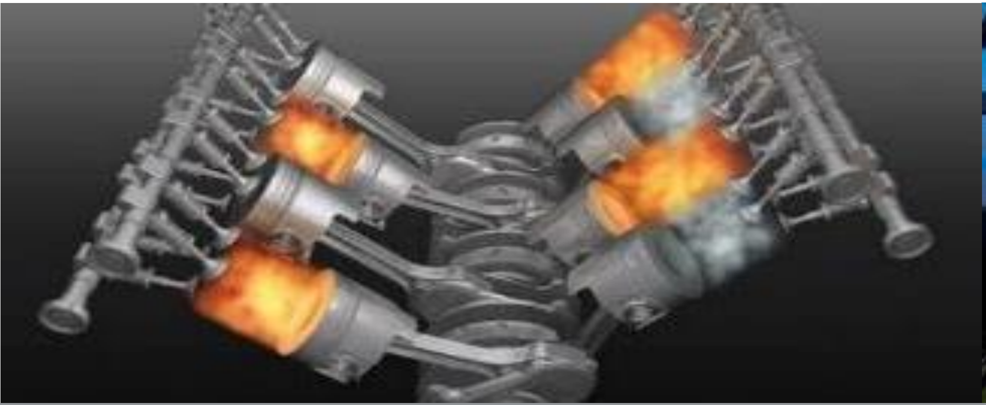


Acknowledgement: This research was conducted as part of the Partnership to Advance Combustion Engines (PACE) sponsored by the U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO). A special thanks to DOE VTO program managers Mike Weismiller and Gurpreet Singh.

Overview

Timeline

- PACE started in Q3, FY19
- PACE will end in FY23 (~25% complete)
- Focus and objectives of individual tasks will be continuously adjusted
- Overall PACE work plan discussed in ACE138

The US government fiscal year (FY) runs from October 1–September 30

Barriers†

USDRIVE Priority 1: Dilute Gasoline Combustion

f. Increase EGR and air dilution tolerance

USDRIVE Priority 3: Low-Temperature Combustion (LTC)

a. Expanded speed and load range

c. Lower combustion noise

d. Simpler transient control/combustion mode switching

Budget‡

Task	FY19	FY20
C.01.01: SNL, Ekoto Advanced Ignition to Enable Alternative Combustion Modes*	$370k	$460k*
F.02.02: SNL, Dec Multi-Mode Combustion Phasing Control	$280k	$280k
G.02.01: ORNL, Kaul Machine Learning (ML) and Deterministic Patterns	$150k	$200k

*The majority of work from task C.01.01 is presented in ACE141: Advanced Ignition System Fundamentals and Simulation

Partners

PACE is a DOE-funded consortium of 6 national laboratories working towards a common goal (ACE138)

- Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, and more

Task-specific partners

- C.01.01 (SNL, Ekoto: Ignition): Argonne National Laboratory, Transient Plasma Systems (TPS), Tennoco, Auburn University, University of Texas
- F.02.02 (SNL, Dec: ACI): Lawrence Livermore National Laboratory (LLNL), SUNY – Stony Brook, Clemson University, ORNL
- G.02.01 (ORNL, Kaul: ML/Nonlinear Dynamics): SNL, Argonne, Lubrizol

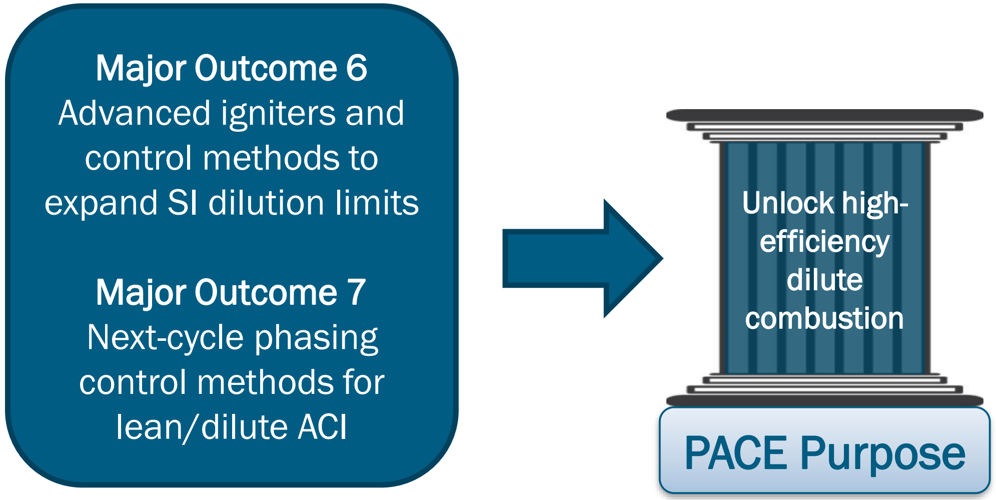
† From USDRIVE Advanced Combustion and Emission Control (ACEC) Tech Team (TT) Roadmap: https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

‡ Full PACE budget breakdown by task is included in reviewer-only slides

Relevance

Overarching PACE Relevance (see ACE138)

- PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.
- Project plan developed in conjunction with USCAR to ensure relevance to stakeholders



Task-Specific Relevance

PACE Major Outcome 6 aims to increase EGR and air dilution tolerance for SI combustion, which is a priority research area in the USDRIVE roadmap to higher-efficiency light duty engines

- Task C.01.01 (SNL, Ekoto) utilizes advanced ignition systems including barrier discharge and nanosecond-pulse plasma igniters to extend the misfire dilution limit
- Task G.02.01 (ORNL, Kaul) aims to extend misfire and partial burn dilution limits through active controls based on identification of recurring dynamical patterns in cyclic variations using nonlinear dynamics analysis and Machine Learning (ML)

PACE Major Outcome 7 aims to address USDRIVE barriers to low-temperature combustion/advanced compression ignition (ACI) including expansion of speed/load range, reduction of combustion noise, and simpler transient control and combustion mode switching

- Task F.02.02 (SNL, Dec) uses double-direct injection (DDI) and other injection strategies to extend the operability range and transient performance of LTC strategies for high-efficiency light-duty (L-D) engines
- Task G.02.01 (ORNL, Kaul) uses ML and nonlinear dynamics analysis to identify deterministic patterns that can be corrected through active controls to extend the LTC operability range

Development of surrogate fuel for use in simulations and experiments contributes to overall PACE progress across many tasks

Milestones

Task	Funding	Description of Milestone or Go/No-Go Decision	Status
C.01.01 (SNL, Ekoto: Ignition)	$460k	12/31/2019: Engine testing of SACI with Corona, BDI, and NRPD LTP igniters for ACEC 1300 rpm 3 bar IMEP reference condition.	Complete
F.02.02 (SNL, Dec: ACI)	$280k	9/30/2020: Work with multi-laboratory team to develop an accurate 7–9 component surrogate for RD5-87 (regular E10), and experimentally validate its performance and the performance of other surrogates for lean/dilute LTGC/HCCI engine combustion.	On Track
		9/30/2020: Complete a study of multiple-injection timings, fuel split between injections, and global equivalence ratio for CA50 control, and demonstration of CA50 control through load sweep – submit paper on results.	On Track
G.02.01 (ORNL, Kaul: ML/Nonlinear Dynamics)	$200k	9/30/2020: Implement machine learning based algorithms for dilute combustion instability prediction, leveraging results from internal ORNL FY19 LDRD project, and evaluate efficacy for enabling next-cycle control to improve stability at the dilute limit.	On Track

Multifaceted Approach to Unlock High-Efficiency Dilute Combustion

Major Outcome 6
Advanced igniters and control methods to expand SI dilution limits

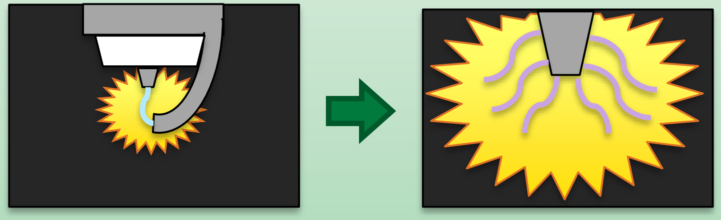
Unlock high-efficiency dilute combustion

PACE Purpose

Major Outcome 7
Next-cycle phasing control methods for lean/dilute ACI

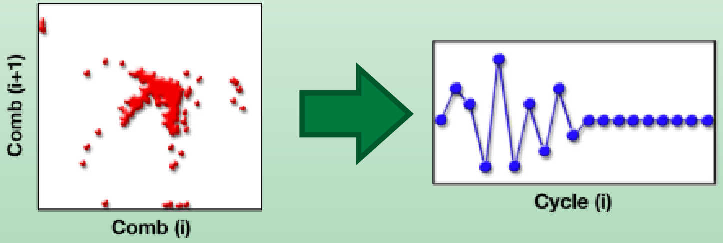
SNL, Ekoto: Ignition

Use advanced low-temperature plasma (LTP) igniters to expand SI dilution limit through the formation of large initial flame kernels



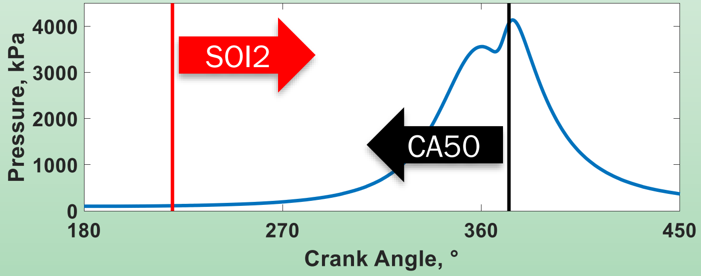
ORNL, Kaul: ML/Nonlinear Dynamics

Use machine learning and nonlinear dynamics to identify and predict recurring patterns and enable next-cycle stability control



SNL, Dec: ACI

Use advanced direct injection control to vary fuel stratification for next-cycle CA50 control of ACI, enabling transient operation

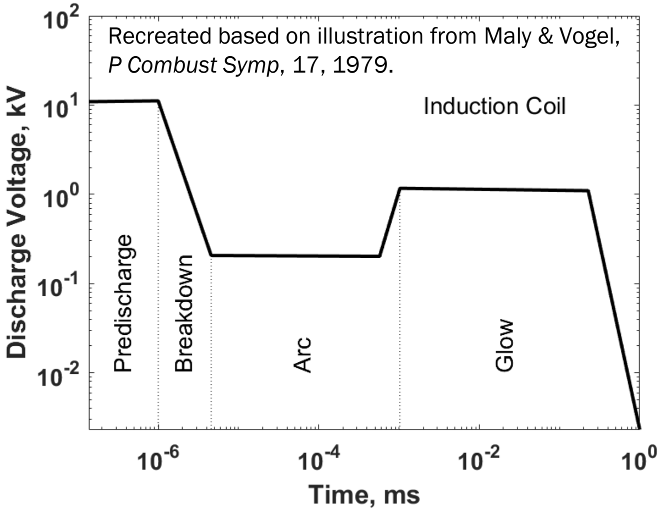


Improved dilution tolerance with advanced low-temperature plasma ignition systems

Motivation: slow early flame development limits homogeneous SI dilution

- High-tumble flows aid flame development but lead to increased heat transfer
- Lean-stratified SI results in unacceptable engine-out NO_x emissions

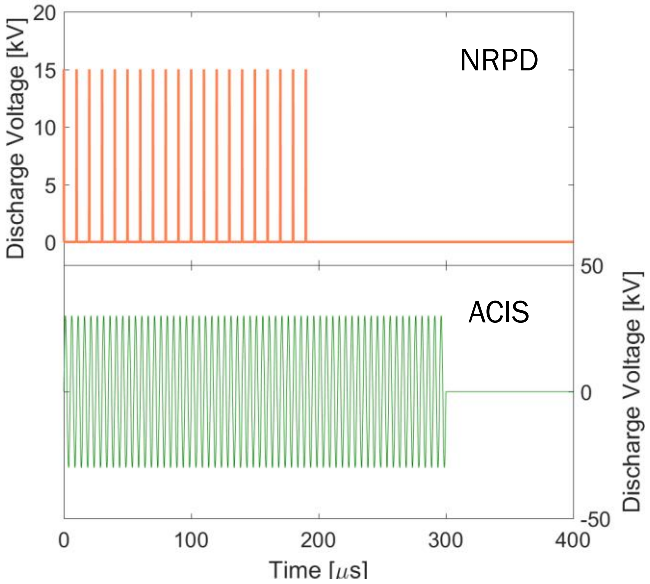
Novel LTP igniters expand dilution tolerance through the formation of large initial flame kernel volumes and active radical species



Compared 3 LTP igniters to spark ignition for lean operation on SG2 engine

- TPS Nanosecond Repetitively Pulsed Discharge (NRPD)
  - Repetitive (10 KHz+), high-voltage (15 kV+) DC ns pulses
  - Strong LTP between pin-to-pin electrodes (modified spark plug geometry)
- Tenneco Advanced Corona Ignition System (ACIS):
  - Radio-frequency (MHz+), high-voltage (20 kV+) discharges
  - High-energy corona streamer propagation into bulk-gas
- Tenneco Barrier Discharge Igniter (BDI)
  - Same ACIS pulse hardware
  - Strong radical formation from surface discharges

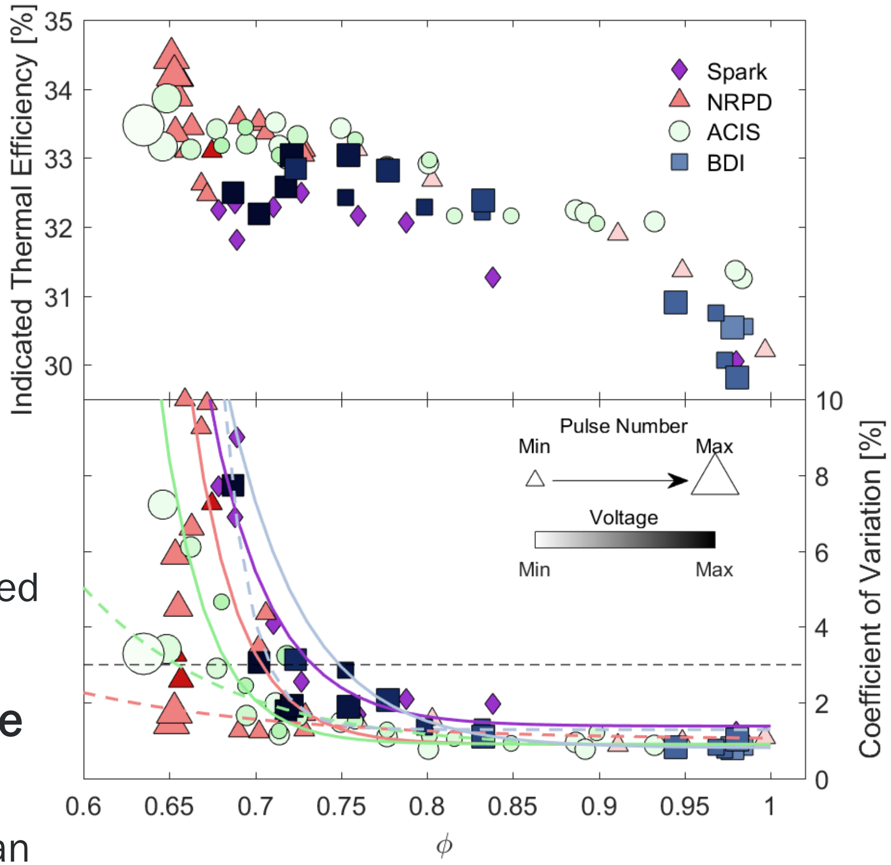
Operation at ACEC 1300 rpm, 3 bar BMEP operating condition

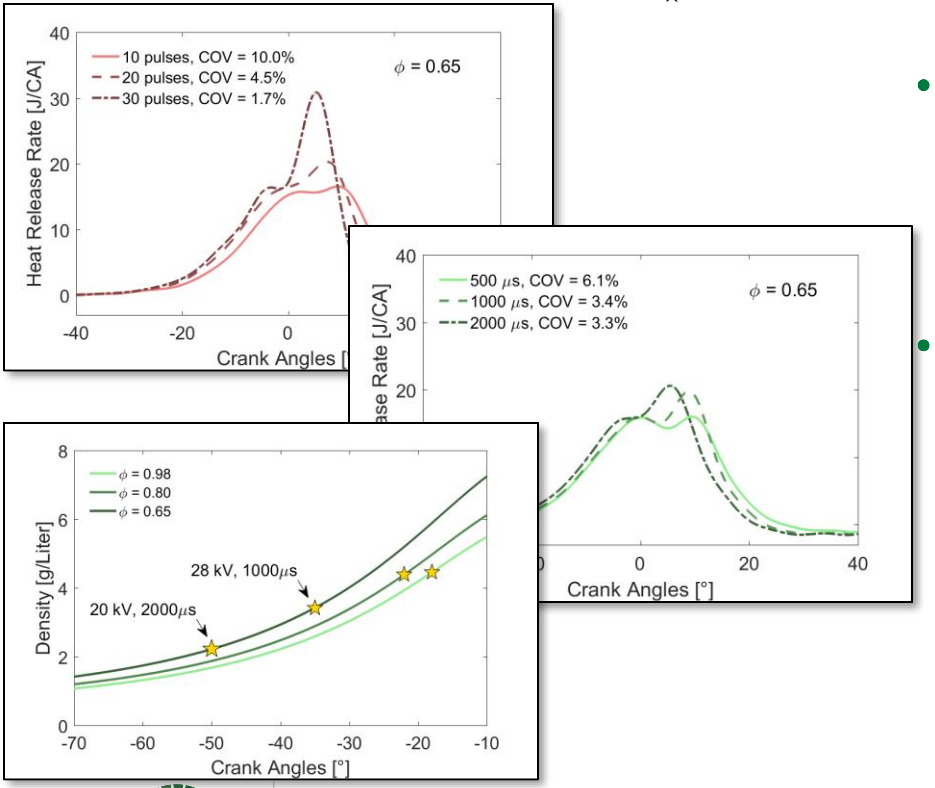


More details available in ACE141: Advanced Ignition System Fundamentals and Simulation

Improved SI lean-limit extension with LTP ignition provided that pulse duration was increased

- Homogeneous lean stability ignition limits extended from ϕ of 0.73 for the spark igniter to 0.68 for ACIS and beyond 0.65 for NRPD
  - No notable lean-limit extension with BDI, although intake prestrikes (previously observed to improve stability) were not used
  - Peak ITE increased from 32.5% for spark to 33.8% for ACIS & 34.4% for NRPD
  - Lean-limit ACIS/NRPD NO_x emissions reduced ~30% relative to lean-limit spark





- Higher NRPD pulse number used to extend lean stability limits
  - Lean-limit never found due to limited test window
- Longer ACIS pulse duration likewise required for lean mixtures
  - Despite higher charge mass for lean mixtures, required spark advance led to lower charge density at ignition timing
  - Discharge voltage/duration was limited by arcing to the injector tip

Planned EGR sweeps and complementary flame kernel imaging deferred until Q4 due to lab shutdown

Characterize, Predict, and Control Chaos

Motivation: SI dilution is limited by cyclic variability due to poor ignitability (misfires) and slow flame propagation (partial burns)

- Chaotic cycle-to-cycle variations: deterministic effects coupled with stochastic variations
- Residual gas composition provides feedforward mechanism for deterministic coupling

Active controls to mitigate instabilities based on next-cycle prediction through ML and/or nonlinear dynamics techniques could extend the SI dilution limit

Characterize deterministic patterns in unstable combustion using Machine Learning (ML) and nonlinear dynamics analysis

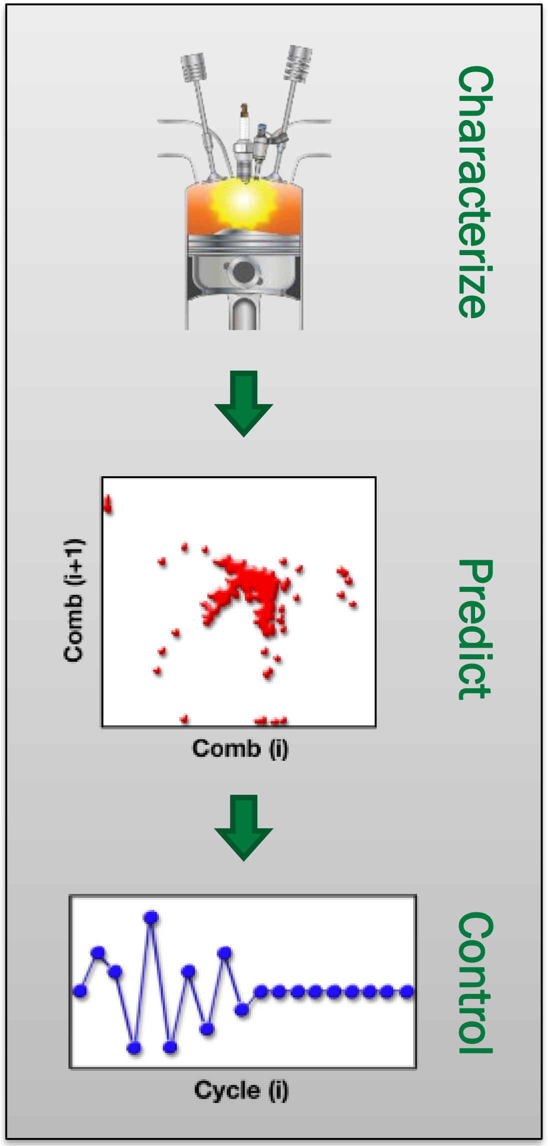
- Identify and characterize dynamics of combustion instabilities at dilute limits
- Enhance understanding of feedback mechanisms

Predict next-cycle dynamics using ML, probabilistic, or model-based methods

- Data interpretation and development of control-oriented models for simulation
- Pattern recognition and prediction through ML and probabilistic techniques

Control strategies developed to mitigate next-cycle combustion instabilities and extend dilute limits

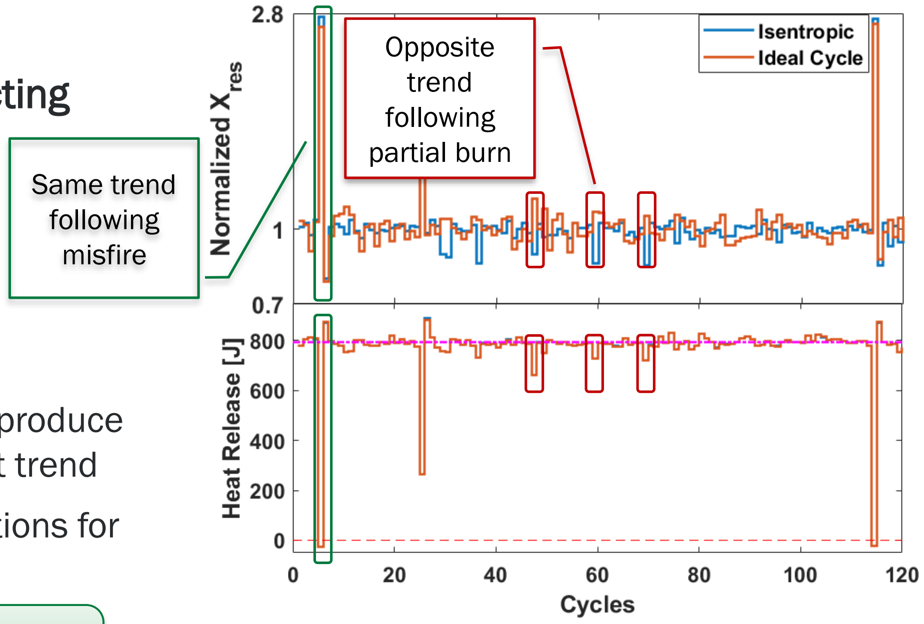
- Take advantage of deterministic features to stabilize combustion
- Leverage machine learning, advanced simulations



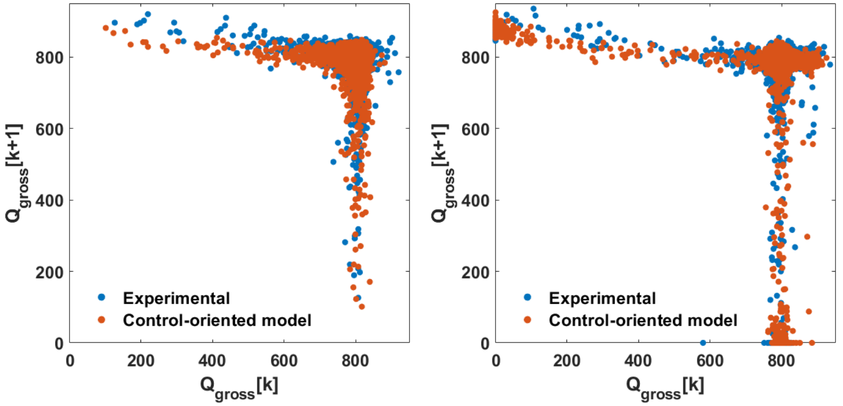
Developed nonlinear-dynamics-based techniques for predicting dilute SI cyclic variability

- An existing model for dilute SI cyclic variability[1] was extended for use in predicting next-cycle dynamics
  - Model tracks residual fuel, air, and inert species to next cycle, with sigmoidal function based on composition predicting combustion efficiency; Gaussian noise on inputs simulates stochastic effects
  - Added dependence of residual gas fraction on prior-cycle combustion event
  - Found that existing methods of estimating residual gas fraction from pressure data produce opposite results following partial burn events: plan to use 1-D CFD to identify correct trend
  - Good agreement between model and experimental dynamics for standalone simulations for both misfire-dominated and partial-burn-dominated operation

Model was then adapted to use prior-cycle engine data in place of internally-tracked variables to enable real-time prediction of next-cycle dynamics



- Symbol sequence statistics used to develop probabilistic prediction of next-cycle dynamics
  - Partition time series data and assign “symbols” to each bin; then build “words” of a chosen number of cycles (sequence length) in a moving window (details in backup slides)
  - Build histogram to identify probability of each possible word in a training data set
  - For sequence length *L*, consider previous *L*-1 cycles and compare to histogram to determine probability of each symbolic value for next cycle through Bayesian inference

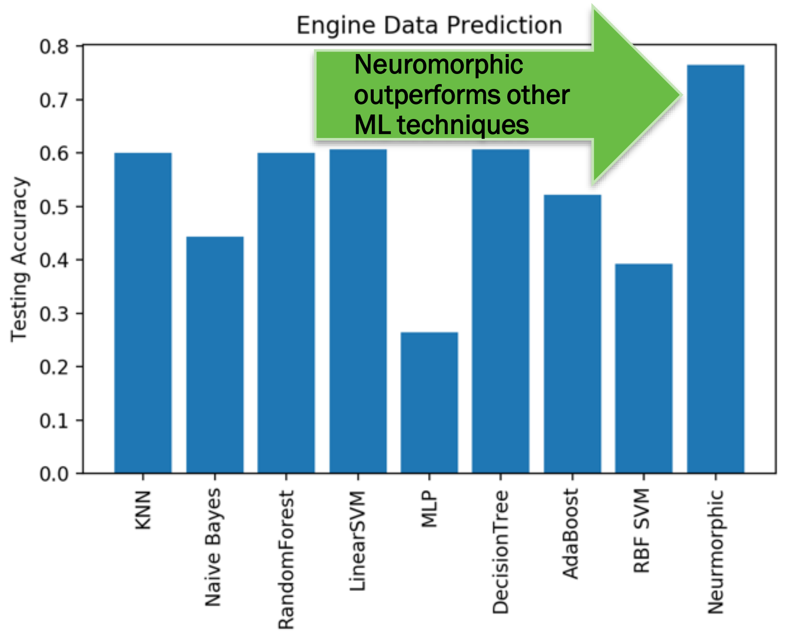


Heat release return maps for operation at 2000 rpm, 4 bar BMEP, 16% EGR with spark timings of 45°BTDC (partial burns dominate) and 70°BTDC (misfires dominate)

1. Daw, C. S.; Finney, C. E. A.; Green, J. B. J.; Kennel, M. B.; Thomas, J. F. & Connolly, F. T. “A Simple Model for Cyclic Variations in a Spark-Ignition Engine” *SAE Technical Paper 962086,* 1996. doi:10.4271/962086

Machine learning offers potential advantages for prediction and control of dilute SI cyclic variability

- **Machine learning approaches applied to predict next-cycle variations**
  - Collaboration with ORNL LDRD project aimed at adapting "EONS" neuromorphic training framework for real-time sensor data analysis
  - ORNL "MENNDL" software utilizes high-performance computing (HPC) resources (Titan, Summit) to optimize design of neural networks for high accuracy, small size, and low power requirements
  - Good potential for low-cost, edge-computing implementation
  - Preliminary results indicate that neuromorphic systems are well-suited to process the engine time series data for prediction
- **Preliminary results show promise for ML approach**
  - Comparison of accuracy in cycle-to-cycle heat release (HR) trend (increase/decrease from prior cycle) shows advantage for ML vs model or symbol sequence approaches
  - ML and model approaches give better resolution of prediction than symbol sequence, which should enable more precise control decisions: important due to highly nonlinear sensitivity of combustion to composition at the dilute limit
  - All methods capture high-energy cycle following misfire but have less success predicting misfire events
    - Best cases are accurately predicting about half of misfires without generating excessive false positives
    - About 3% of cycles in test data set were misfires: predictions are significantly better than random guessing, though not yet as good as desired
  - Prediction of dynamics for partial burns is much better, as indicated by higher accuracy of predicted next-cycle trend: may expect best performance at partial-burn dilution limit

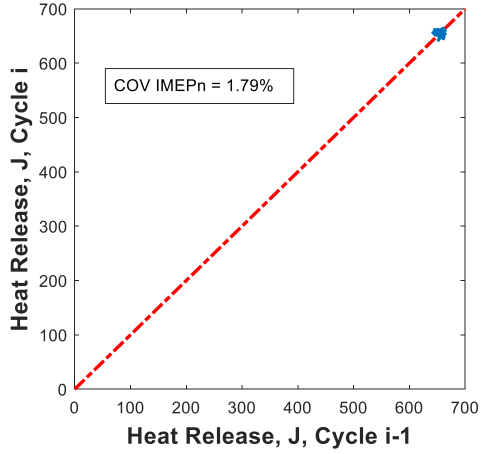


Prediction method	Accuracy of HR trend
Model	69%
Symbol Sequence	73%
Machine Learning	75%

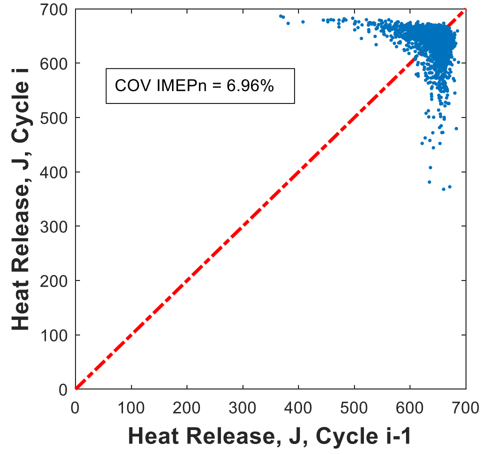
Distinction between partial-burn and misfire dilution limits and impact of combustion phasing is described in technical backup slides

ACI data at combustion stability limits show evidence of deterministic influence on cyclic variations

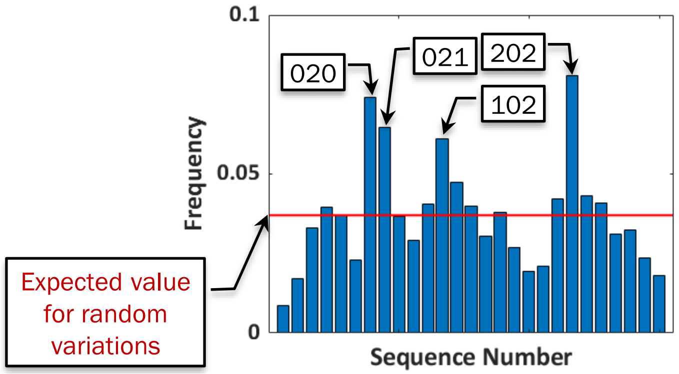
- Data collected at retarded combustion phasing during double direct injection (DDI) load sweep at SNL
- Dynamics are similar to dilute SI cyclic variations at partial-burn dilution limit
  - Return map shows characteristic “boomerang” shape
    - Negative slope on upper arm indicates anti-correlation for energy released in cycle following a low-energy cycle
    - Time-asymmetry (asymmetry about 45° diagonal) implies deterministic behavior
  - Symbol sequence histograms show significant patterns of high-low-high energy cycles
    - Occurrence more frequently than expected value for random cycles indicates non-random, deterministic behavior
    - Implies deterministic coupling is likely primarily through residual fuel/composition rather than temperature effects
    - More complex patterns observed with longer sequence lengths
- Initial results indicate further investigation is warranted to determine feasibility of mitigation through active control
  - Larger data sets will allow exploration of ML approaches



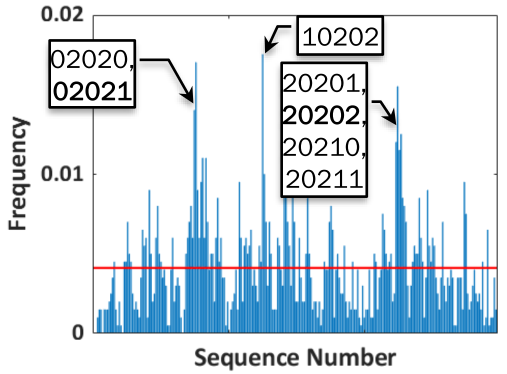
Heat release return map for stable combustion
1200 rpm, 3.6 bar IMEPn, φ=0.33,
CA50 8°ATDC, RI 1.67 MW/m²



Heat release return map for unstable combustion
1200 rpm, 3.4 bar IMEPn, φ=0.33,
CA50 12°ATDC, RI 0.27 MW/m²



Symbol sequence histogram for unstable combustion at 1200 rpm, 3.4 bar IMEPn with 3 partitions and 3-cycle sequence length



Symbol sequence histogram for unstable combustion at 1200 rpm, 3.4 bar IMEPn with 3 partitions and 5-cycle sequence length

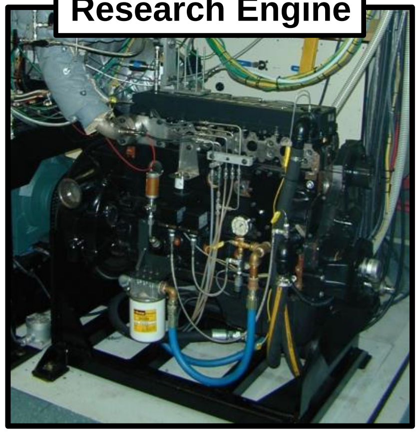
CA50 control for L-D ACI using variable fuel stratification

Motivation: Transient response in low-temperature gasoline combustion (LTGC)/advanced compression ignition (ACI) operation requires fast (next-cycle) control authority

- Intake T influences ignition and phasing, but cannot be changed rapidly
- Boost pressure also subject to filling/emptying dynamics and not next-cycle capable

Direct injection strategies are next-cycle capable, enabling transient CA50 control

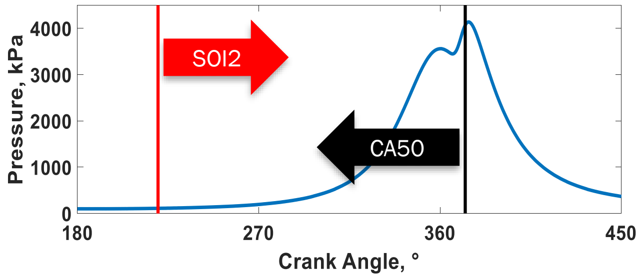
Sandia LTGC/ACI Research Engine



Double-direct injection (DDI) strategy used to produce partial fuel stratification (PFS)

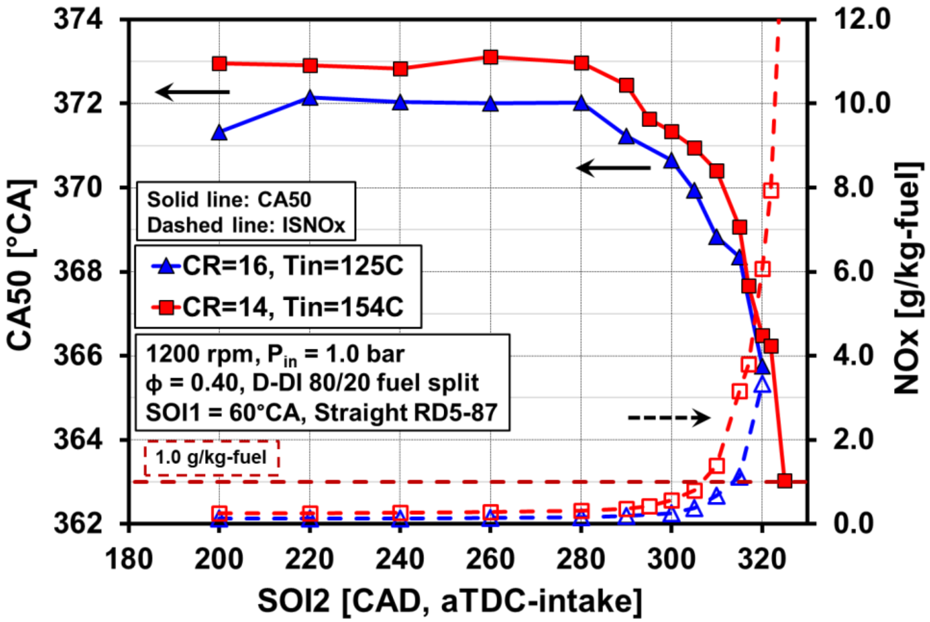
- Inject 70-80% of fuel early in intake stroke for homogeneous charge mixture
- Inject remaining 20-30% of fuel during compression stroke to produce stratification
- Vary late-DI timing (SOI2) to vary stratification and thus control CA50

1) Quantify range of CA50 control authority with DDI-PFS at fixed loads
2) Evaluate ability of DDI-PFS to control CA50 in load sweep with constant T-intake
3) Investigate potential of late single-DI (S-DI) to expand low-load control map
   - Vary S-DI timing to control CA50 via fuel stratification

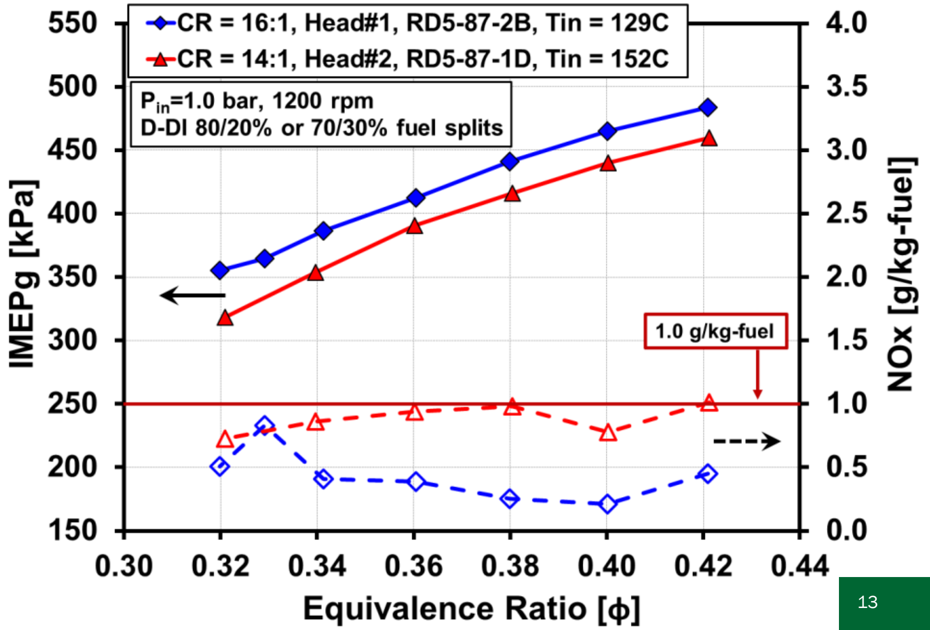


DDI-PFS controls CA50 through load sweeps with constant T_{in}

- **DDI-PFS can control CA50 over a wide range** ⇒ even at naturally aspirated (P_{in}= 1 bar) conditions where RD5-87 is only mildly ϕ-sensitive.
  - CA50 adv. as SOI2 retarded: richer regions ignite faster due to ϕ-sensitivity
  - Due to low ϕ-sensitivity of RD5-87 at these conditions, must retard SOI2 > 280 CAD to stratify sufficiently to advance CA50
  - NO_x remains very low except latest SOI2s ⇒ lower with CR=16
  - **Control authority 8–10 CAD**



- **DDI-PFS controls CA50 for good performance through load sweeps with both CRs.**
  - For CR = 16, IMEPg = 484 → 355 kPa (> 30% change above idle)
  - For CR = 14, IMEPg = 460 → 319 kPa (> 35% change above idle)
  - NO_x < 1.0 g/kg-fuel ⇒ PM < 0.028 g/kg-fuel (typically ~0.005 g/kg-fuel)



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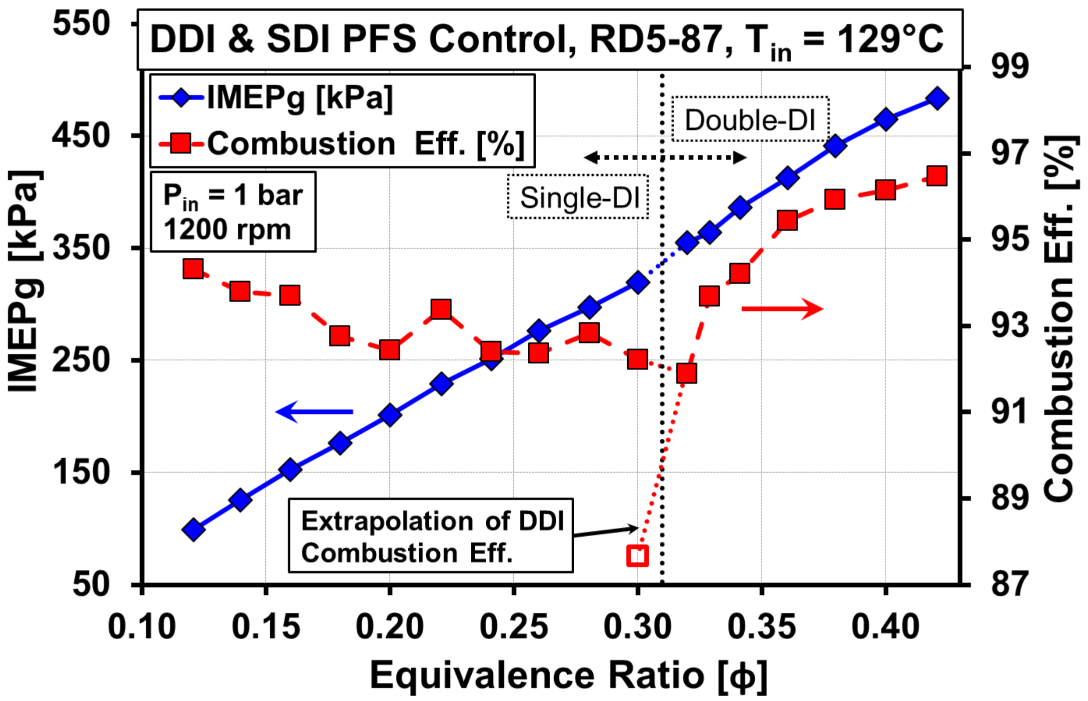
Combined DDI/S-DI strategy extends low-load performance

Can the control range of LTGC/ACI using stratification be increased with an alternative injection strategy at lower loads? Investigate CR=16 only.

- Extending DDI-PFS control to low loads (ϕ < ~0.32) is limited by a significant drop in combustion efficiency ⇒ Fueling in first DI becomes so low CO-to-CO_2 reactions not complete.
- **For lower loads, switch to retarded single-DI (S-DI) fueling** to keep local ϕs sufficiently high for complete combustion.
  - As ϕ reduced from 0.30 to 0.12, increase stratification by retarding SOI for S-DI fueling from 315 to 345 CAD to maintain good combustion efficiency, good stability, and low noise.



- **Stratification with retarded S-DI fueling provides good low-load performance without additional heating.**
- Combining DDI and S-DI PFS allows CA50 control for a large change in load ⇒ 99 ≤ IMEPg ≤ 484 kPa with T_{in} = constant.
  - These techniques can provide next-cycle control
  - NOx is very low for D-DI control, < 0.8 g/kg-fuel ⇒ NOx higher for S-DI control, but still relatively low
  - **PM is very low at all points, < 0.026 g/kg-fuel**

Development of new PACE surrogate for RD5-87 gasoline

Motivation: Surrogate needed for simulations and controlled experiments across all relevant operating conditions, capturing physical and chemical properties

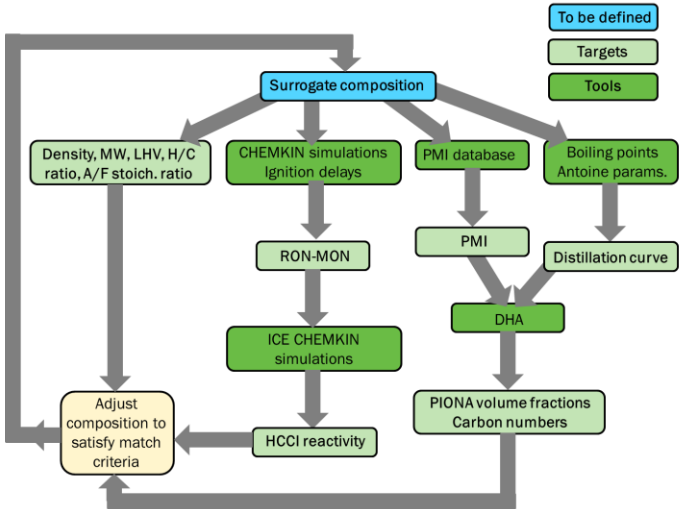
- Research Octane Number (RON) & Motor Octane Number (MON)
- LTHR & ITHR autoignition
- Particulate Matter Index (PMI)
- Distillation curve
- Dilute operation
- Boosted operation
- Various thermal conditions

Collaborate with LLNL to develop a surrogate for RD5-87 (regular E10 gasoline) valid for all PACE experiments and simulations (sprays, combustion, emissions)

- Conduct engine tests of surrogates to measure low- and intermediate-temperature heat release (LTHR & ITHR) and dilute autoignition to ensure that they match those of RD5-87
- Use engine test data to validate & improve both surrogate compositions & kinetic models

Iterative approach to design new surrogate blends at SNL

- Initial composition guided by detailed hydrocarbon analysis (DHA) of RD5-87
- Use CHEMKIN simulations with LLNL Co-Op mechanism to tune surrogate composition to
  - Match LTHR, ITHR, and dilute autoignition timing
  - Match RON & MON in simulated tests
- Engine experiments and formal RON & MON measurement to test surrogate performance
- Initial CHEMKIN results showed errors in match to engine data and RON & MON
  $\Rightarrow$ Offset CHEMKIN targets to compensate for errors & re-tune surrogate composition
- **Obtained very close match to RON and MON of full distillate RD5-87 in one iteration**

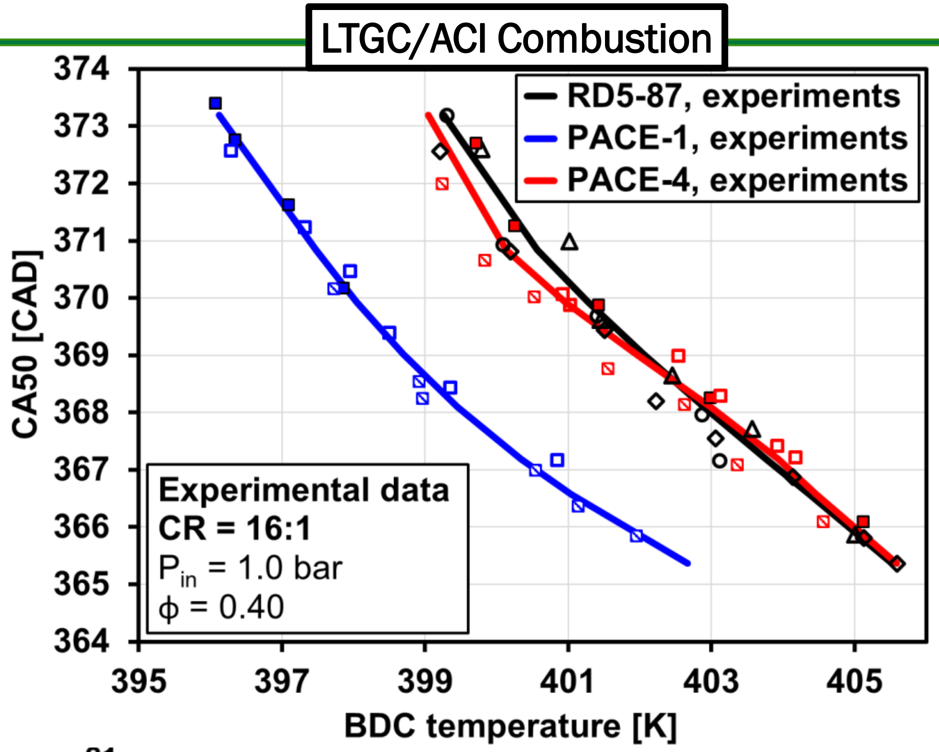


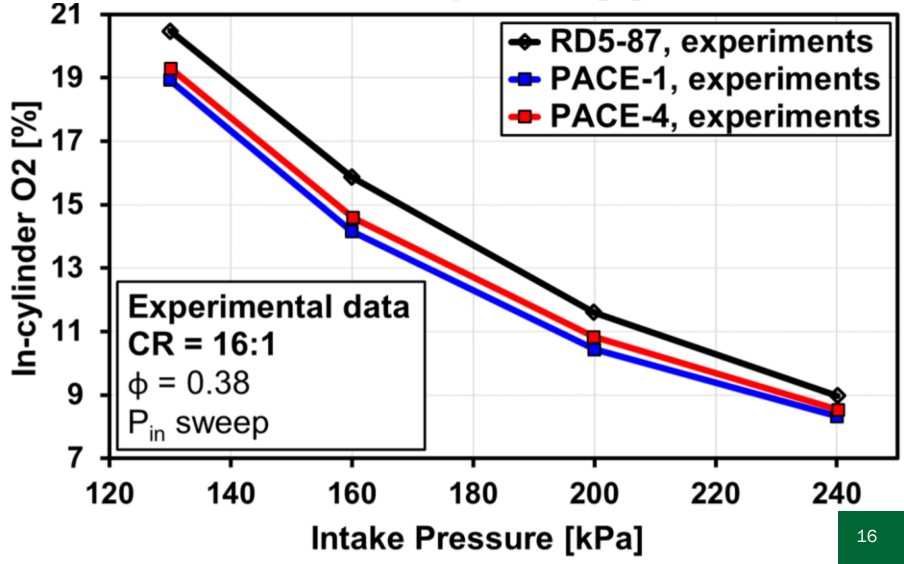
This report details SNL contributions. Overview of PACE surrogate development efforts presented in ACE139: Development of an Optimized Gasoline Surrogate Formulation for PACE Experiments and Simulations

PACE-4 Surrogate matches RD5-87 autoignition properties well for P_{in} = 1 bar

- **Starting point:** Previous work at Sandia in consultation with LLNL led to the **SNL-LLNL surrogate** (7-components).
  - First surrogate matched dilute ACI autoignition reactivity of RD5-87, but it did not replicate PMI & distillation curve.
- **Tested initial PACE surrogate, PACE-1:** matched PMI & distillation, but SNL engine tests showed:
  $\Rightarrow$ too reactive for ACI autoignition, at both P_{in}= 1 bar and boosted.
- **Designed PACE-4 surrogate at SNL** to better match ACI autoignition.
  - Apply CHEMKIN simulations w/ LLNL mech. $\Rightarrow$ match ACI autoignition and simulated RON & MON tests (Westbrook's method).
  - Match PMI & distillation curve $\Rightarrow$ NREL method and NIST REFPROP.
- **PACE-4 experimentally tested in Sandia LTGC/ACI research engine:**
  - Matches RD5-87 autoignition well at P_{in} = 1 bar.
  - Still overly reactive for boosted ACI.
  - Neither PACE-1 nor PACE-4 match measured RD5-87 RON & MON.

	RON	MON
RD5-87	92.3	84.6
PACE-1 (measured)	91.8	92.8
PACE-4 (measured)	93.6	83.6

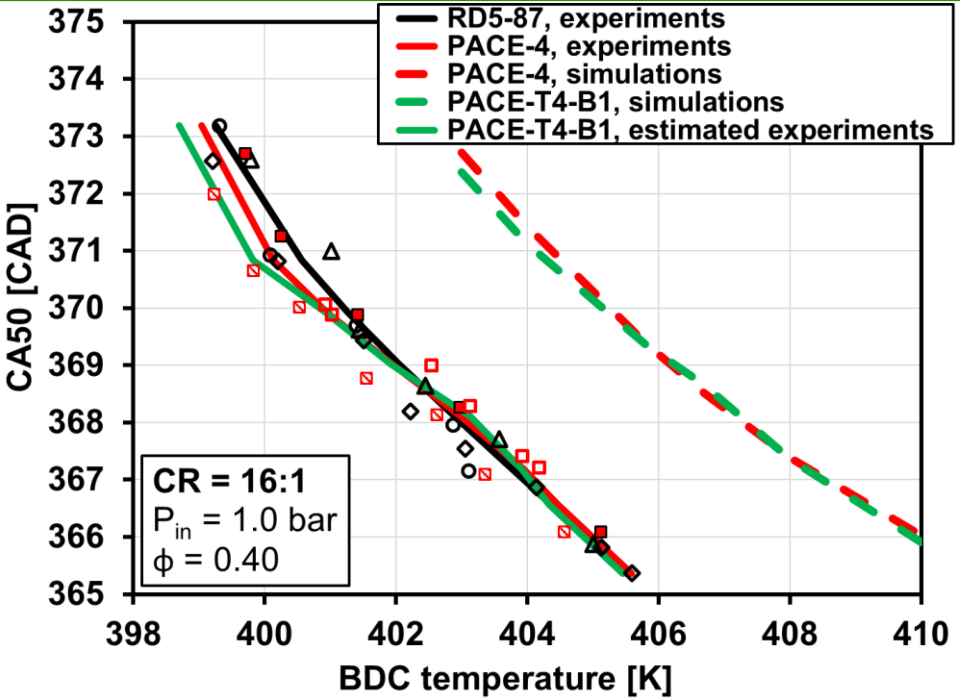


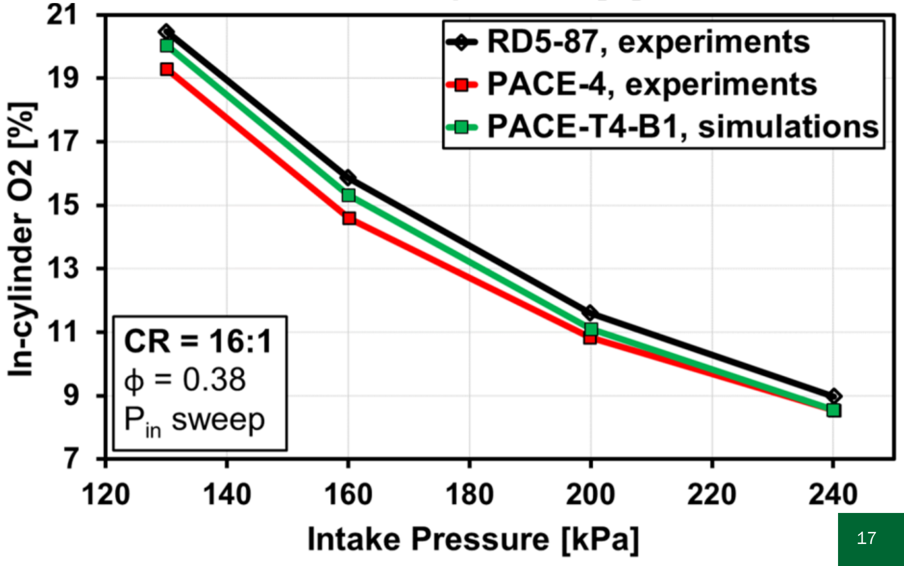


PACE-T4-B1 surrogate improves match for distillation, RON & MON, & boosted autoignition performance

- Difficult to improve PACE-4 performance with the existing palette of surrogate components ⇒ **over-constrained problem**
  ⇒ **Tetralin** added due to high PMI & boiling point (still 9 components).
- **PACE-T4-B1** designed for closer match to DHA by including tetralin.
- **PMI & distillation curve** of surrogate match RD5-87's PMI and high-end of the distillation curve by adding just 2.5% tetralin.
- **Autoignition reactivity:** Simulations of PACE-4 experiments show that the model under-predicts the reactivity of the fuel.
  - Offset applied to PACE-T4-B1 simulations to compensate for model error & estimate the experimental reactivity at naturally aspirated conditions.
  - Simulations suggest better match at intake-boosted conditions.
- **RON & MON:** offsets applied to simulated RON & MON tests based on PACE-4 measurements (SwRI).
  - **Measurements show an excellent match between PACE-T4-B1 and RD5-87 for both RON and MON.**

	RON	MON
RD5-87	92.3	84.6
PACE-T4-B1	92.1	84.5
PACE-4	93.6	83.6





PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Responses to Reviewer Comments

Task C.01.01 (SNL, Ekoto: Ignition)

- **"… investigate the links between faster reaction rates seen with the advanced ignition technologies and how that translates to BTE …"**
  - In FY20, we directly evaluated various LTP igniters (ACIS, BDI, NRPD) at a common part-load operating point (1300 rpm, 3.5 bar IMEP) for an equivalence ratio sweep. Shorter early burn durations by the ACIS and NRPD igniters improved ITE by 0.5–1 points, with an additional 1–1.5 point improvement due an extension of the lean-combustion stability limit.
- **"… recommend that the project team continue to focus on approaches with a strong pathway to commercialization, namely stoichiometric, highly dilute combustion."**
  - It was our intention to likewise evaluate the EGR dilution tolerance limits with the LTP igniters, but this was not possible given the shutdown. These measurements will be prioritized once we are able to get back into the lab.

Task G.02.01 (ORNL, Kaul: ML/Nonlinear Dynamics)

- **This task has not been previously reviewed**

Task F.02.02 (SNL, Dec: ACI)

- **Our early surrogate development work was reported in 2018, and a reviewer commented "An improved surrogate for regular E10 has been developed. Both this surrogate and the LLNL kinetic model seem to work well."**
  - We appreciate this comment regarding our earlier work to develop the SNL-LLNL surrogate mentioned as the starting point for the current effort. This earlier surrogate matched LTGC/ACI autoignition of RD5-87 well, but not other properties. Here we are building on the techniques use previously to develop a surrogate that matches all properties of RD5-87 relevant to PACE studies.
- **An initial investigation of DDI-PFS to control CA50 was reported previously, but there were no direct reviewer comments.**

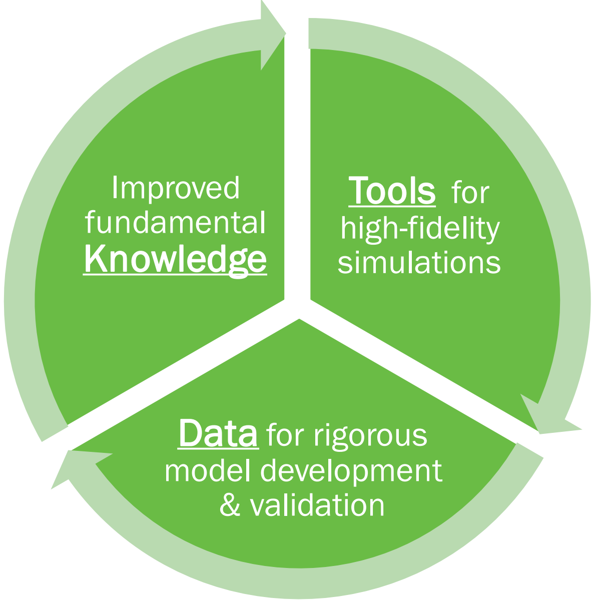
Collaboration

Overall PACE Collaborations (see ACE138)

- PACE is a collaborative project of multiple national laboratories that combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions
- The work plan for PACE is developed in coordination with the USDRIVE Advanced Combustion and Emission Control Tech Team

Task-Specific Collaborations

- Task C.01.01 (SNL, Ekoto: Ignition)
  - Transient Plasma Systems (TPS) and Tenneco: igniter hardware
  - Argonne National Laboratory: plasma modeling
  - TPS/ANL FOA: develop BDI using TPS pulse generators
  - Auburn University and University of Texas FOA: develop better plasma kinetics
- Task G.02.01 (ORNL, Kaul: ML/Nonlinear Dynamics)
  - SNL, Argonne: collaboration on data sets for analysis
  - Lubrizol: collaboration on data set for high-load abnormal combustion analysis (pre-ignition)
- Task F.02.02 (SNL, Dec: ACI)
  - LLNL (McNenly, Pitz, Wagnon): RD5-87 surrogate & kinetic mechanism development
  - SUNY – Stony Brook: CFD to study in-cylinder fuel distributions with DDI-PFS used for CA50 control
  - Clemson University: CFD to study stratification at low loads for improved combustion efficiency and CA50 control
  - ORNL (Kaul): analysis of ACI instabilities



Remaining Challenges and Barriers Proposed Future Research

Any proposed future work is subject to change based on funding levels.

Task	Remaining Challenges and Barriers*	Proposed Future Research
C.01.01 (SNL, Ekoto: Ignition) Major Outcome 6	• BDI: Igniter durability and improved understanding of pre-strike impact • ACIS: Arc avoidance • NRPD: Arc avoidance, improved impedance matching to maximize energy deposition, and minimization of EMI	• Couple BDI with a pre-chamber • Pre-strikes with BDI to improve performance • Flame kernel imaging in the engine for all igniters • Multi-cylinder engine testing
G.02.01 (ORNL, Kaul: ML/Nonlinear Dynamics) Major Outcomes 6 & 7	• Control strategies will need to be devised to take advantage of predictions to mitigate instabilities • Need to develop larger data sets for ML training • Misfire prediction remains challenging	• Develop and implement control strategies to mitigate combustion instabilities based on ML &/or model-based predictions • Further analysis and exploration of ML techniques for next-cycle prediction of ACI combustion instabilities
	This task is cross-cutting, and future work plans include contributions to other PACE outcomes in addition to enabling dilute combustion.	
Major Outcomes 2 & 8	• Applicability of ML and nonlinear dynamics to mitigating other abnormal combustion phenomena remains unknown	• Evaluate the applicability of these techniques to mitigate cold-start combustion instabilities and high-load abnormal combustion phenomena (knock/pre-ignition)
F.02.02 (SNL, Dec: ACI) Major Outcome 7	• Development of new or improved stratification techniques for good combustion efficiency at low loads with lower NO_x • Improved techniques for transient control of ACI • Improved skeletal chemical-kinetic mechanisms for LES-CFD simulations • Further validation and improvement of fuel surrogates	• Explore additional methods of stratification to improve ACI control and extend operating range, while maintaining low NO_x • IR imaging of fuel distributions with DDI-PFS and late Single-DI fueling at low loads in the optical engine to validate CFD modeling and improve fuel stratification techniques, particularly for improved low-load operation and CA50 control • Continue university collaborations on CFD simulations of fuel stratification techniques. Both IR imaging and metal engine data will be used to validate and improve CFD results. Improve skeletal mechanisms and provide them to universities and other national labs. • Evaluate the new SNL PACE-T4-B1 surrogate and new surrogates from LLNL for ACI autoignition reactivity in the SNL ACI engine $\Rightarrow$ Further adjust surrogate compositions and re-test as necessary

* PACE-wide barriers are discussed in ACE138

Summary

Any proposed future work is subject to change based on funding levels.

Relevance

- Overall goals of PACE are to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions
- These tasks directly address USDRIVE research priority 1: Dilute Gasoline Combustion and priority 3: Low-Temperature Combustion (LTC)
  - Increase EGR and air dilution tolerance for dilute SI combustion
  - Expanded speed and load range, lower combustion noise, and simpler transient control/combustion mode switching for LTC combustion
- Accurate surrogate for RD5-87 will enable PACE simulations and collaborative experiments across all objectives

Approach

- Address SI dilution limits through advanced LTP igniters and control of cyclic variations leveraging ML/nonlinear dynamics predictions
- Develop surrogate for RD5-87 matching relevant properties using iterations of chemical kinetic simulations and experimental validation
- Improve transient control of LTC through DDI/PFS strategy and extend stability limits by leveraging ML/nonlinear dynamics predictions

Accomplishments

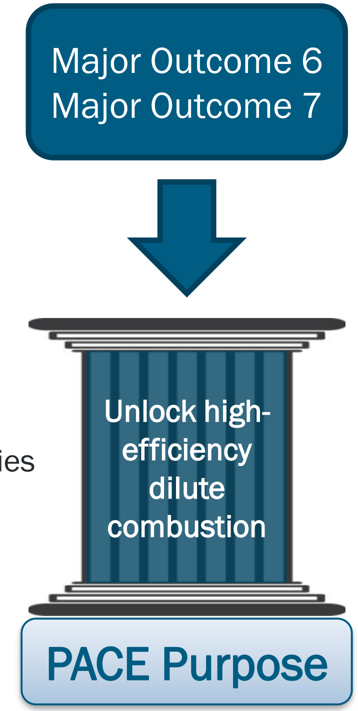
- Demonstrated extension of lean limit with ACIS & NRPD igniters and elucidated impact of pulse-control strategy
- Developed next-cycle prediction methods for dilute SI cyclic instabilities using ML and nonlinear dynamics approaches
- Developed improved PACE-T4-B1 surrogate matching RD5-87 physical properties and combustion performance
- Demonstrated capability for transient control of CA50 for LTGC/ACI at for a load range of 99–484 kPa IMEPg using DDI/late S-DI injection strategies
- Determined that LTGC/ACI combustion instabilities for late combustion phasings exhibit deterministic cycle-to-cycle coupling

Collaborations

- PACE is a collaboration of 6 national laboratories; work plan developed considering input from ACEC TT, code developers, and more
- PACE projects presented at AEC semi-annual program review meeting
- External collaborations with Tenneco, TPS, Lubrizol, and university partners

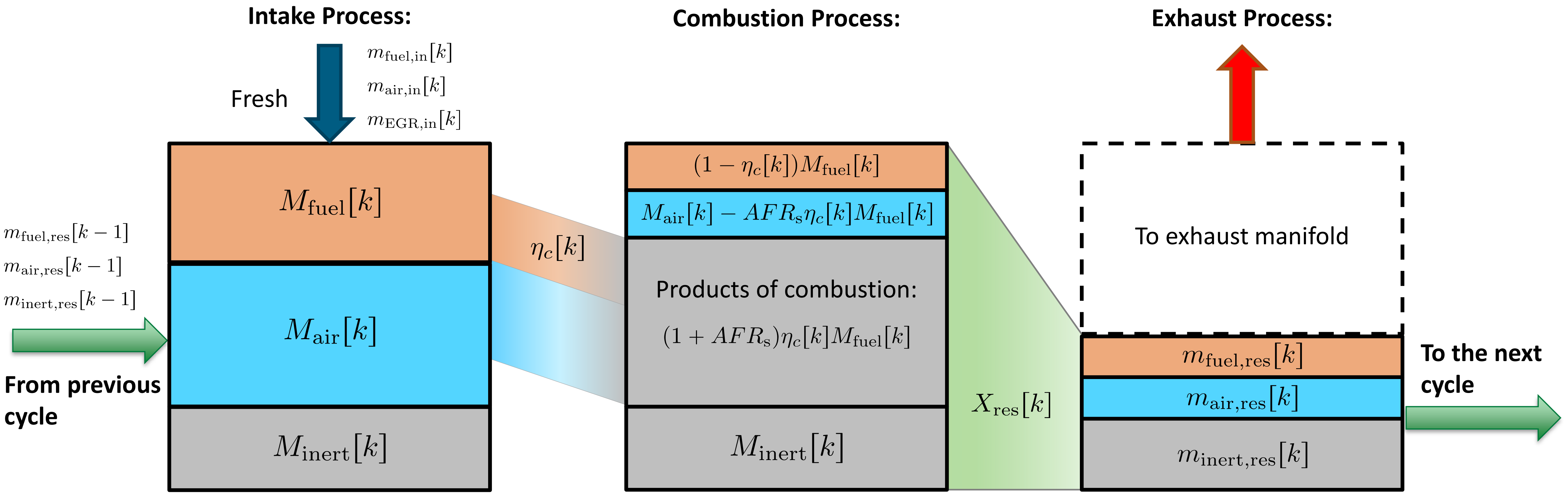
Future Work

- Couple BDI with pre-chamber, explore BDI pre-strikes to improve performance; flame kernel imaging and multi-cylinder engine tests for igniters
- Develop control strategies for mitigation of combustion instabilities through ML/nonlinear dynamics predictions; evaluate applicability to high-load abnormal combustion
- Evaluate new SNL PACE-T4-B1 surrogate for RD5-87 in the SNL ACI engine and new surrogates from LLNL, improve surrogates and iterate as needed
- Continue development of PFS techniques through CFD modeling collaborations and IR imaging of fuel distribution for DDI and late S-DI strategies in the optical engine



Technical Backup Slides

Modeling cycle-to-cycle dynamics of combustion events during EGR-dilution



$$
\begin{aligned}
M_{\text{fuel}}[k] &= m_{\text{fuel,in}}[k] + m_{\text{fuel,res}}[k-1] \\
M_{\text{air}}[k] &= m_{\text{air,in}}[k] + m_{\text{air,res}}[k-1] \\
M_{\text{inert}}[k] &= m_{\text{EGR,in}}[k] + m_{\text{inert,res}}[k-1]
\end{aligned}
$$

$$
\begin{aligned}
\lambda'[k] &= \frac{M_{\text{air}}[k] + M_{\text{inert}}[k]}{M_{\text{fuel}}[k]} \cdot \frac{1}{AFR_{\text{s}}} \\
\eta_c[k] &= f\left(\lambda'[k]\right) \\
Q_{\text{HR}}[k] &= \eta_c[k] M_{\text{fuel}}[k] Q_{\text{LHV}}
\end{aligned}
$$

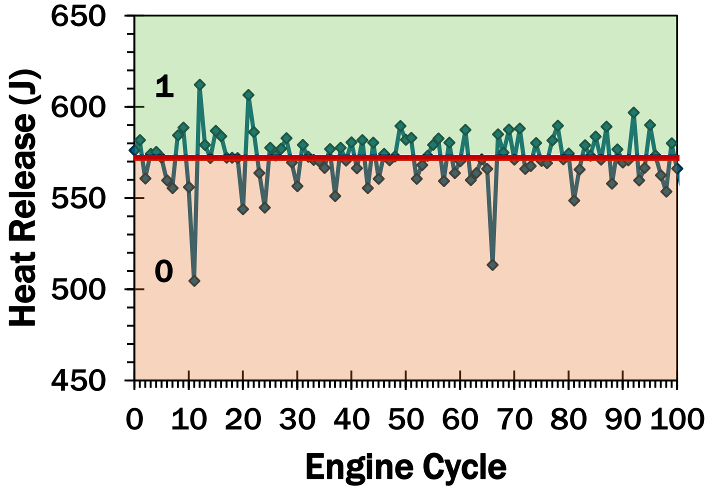
$$
\begin{aligned}
m_{\text{fuel,res}}[k] &= X_{\text{res}}[k](1-\eta_c[k])M_{\text{fuel}}[k] \\
m_{\text{air,res}}[k] &= X_{\text{res}}[k](M_{\text{air}}[k] - AFR_{\text{s}}\eta_c[k]M_{\text{fuel}}[k]) \\
m_{\text{inert,res}}[k] &= X_{\text{res}}[k](M_{\text{inert}}[k] + (1+AFR_{\text{s}})\eta_c[k]M_{\text{fuel}}[k])
\end{aligned}
$$

Key variables to identify from data: $X_{\text{res}}[k], \eta_c[k]$

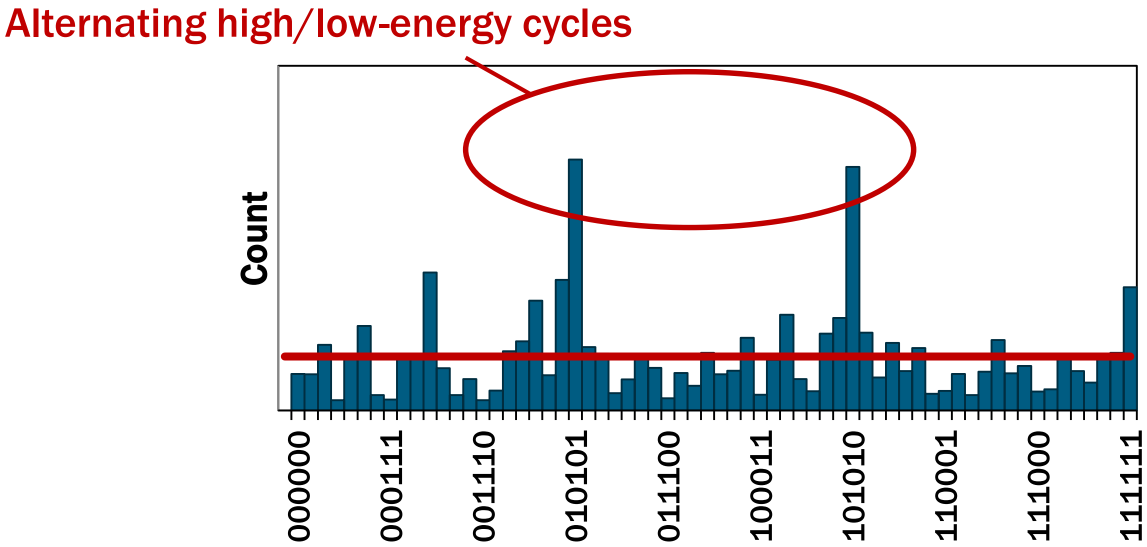
PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Symbol-sequence statistics analysis finds order in chaos

- **Method:**
  - Partition data into discrete bins
    - Each bin is labeled with a "symbol" or "letter"
  - Identify sequences of a given number of cycles
    - These symbol sequences can be thought of as "words" made up of the symbolic "letters"
  - Detect patterns by identifying words that occur frequently
- **This information can be used to better understand dynamics and potentially enable online control of cyclic variability**



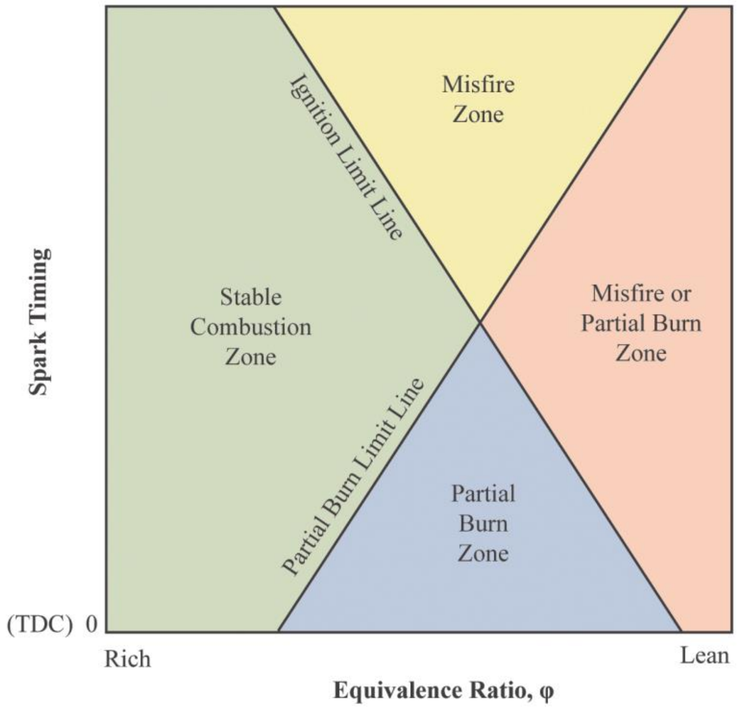
Example time series with binary symbol partition



Symbol sequence histogram with 2 symbolic letters and a word length of 6 cycles

Dilute SI combustion has bimodal limits: partial burn or misfire

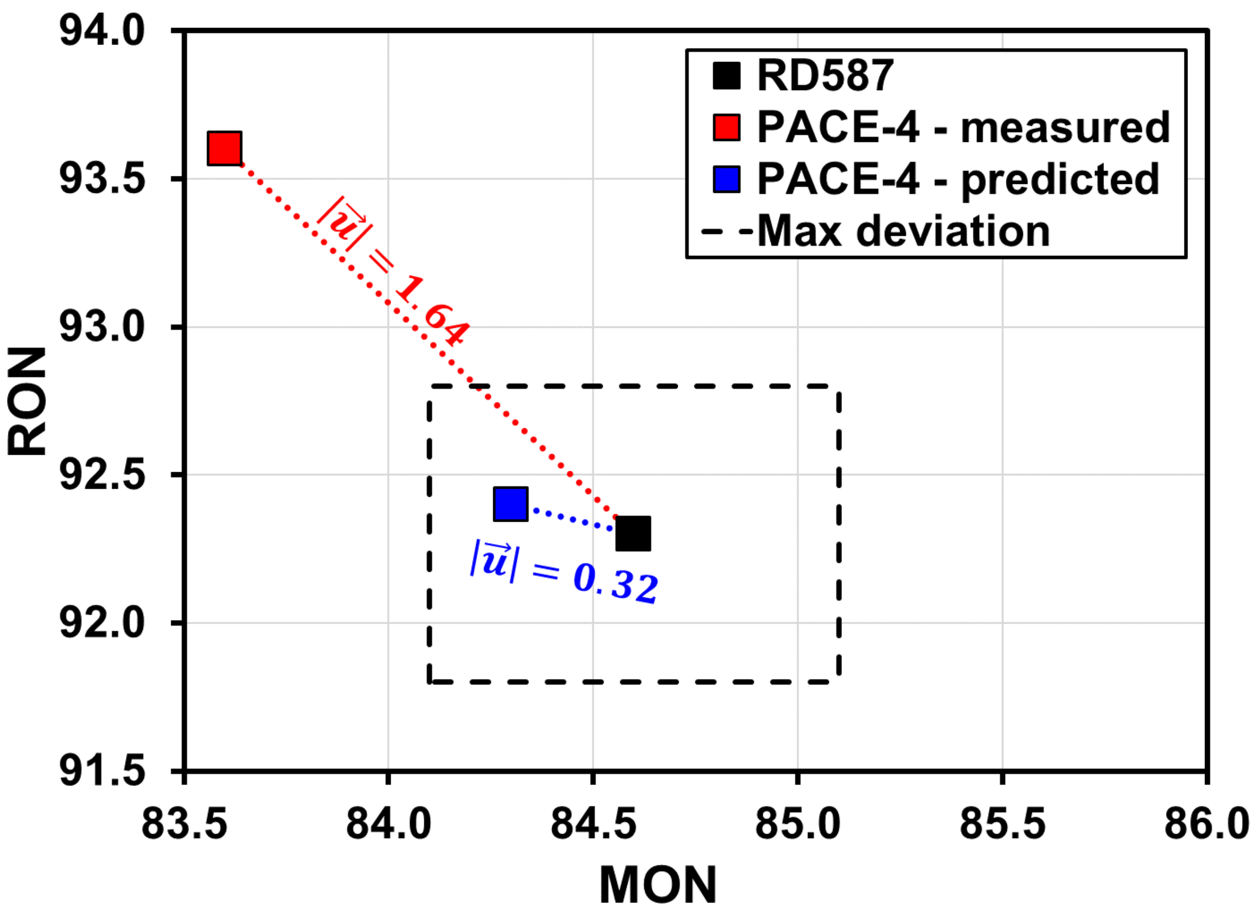
- Bimodal dilute limit, based on spark timing was noted by Quader[1]
- For advanced combustion phasing, ignition (misfire) limit is reached: flame kernel fails to form or is quenched
- For retarded combustion phasing, partial burn limit is reached: combustion begins but is too slow to finish before being quenched via expansion or exhaust valve opening
- Dynamics of cycle-to-cycle variations are different for partial burns vs misfires
  - Same cycle-to-cycle coupling through residual gas composition exists
  - Misfire occurrence highly dependent on stochastic effects of local mixture preparation and turbulence near the spark plug



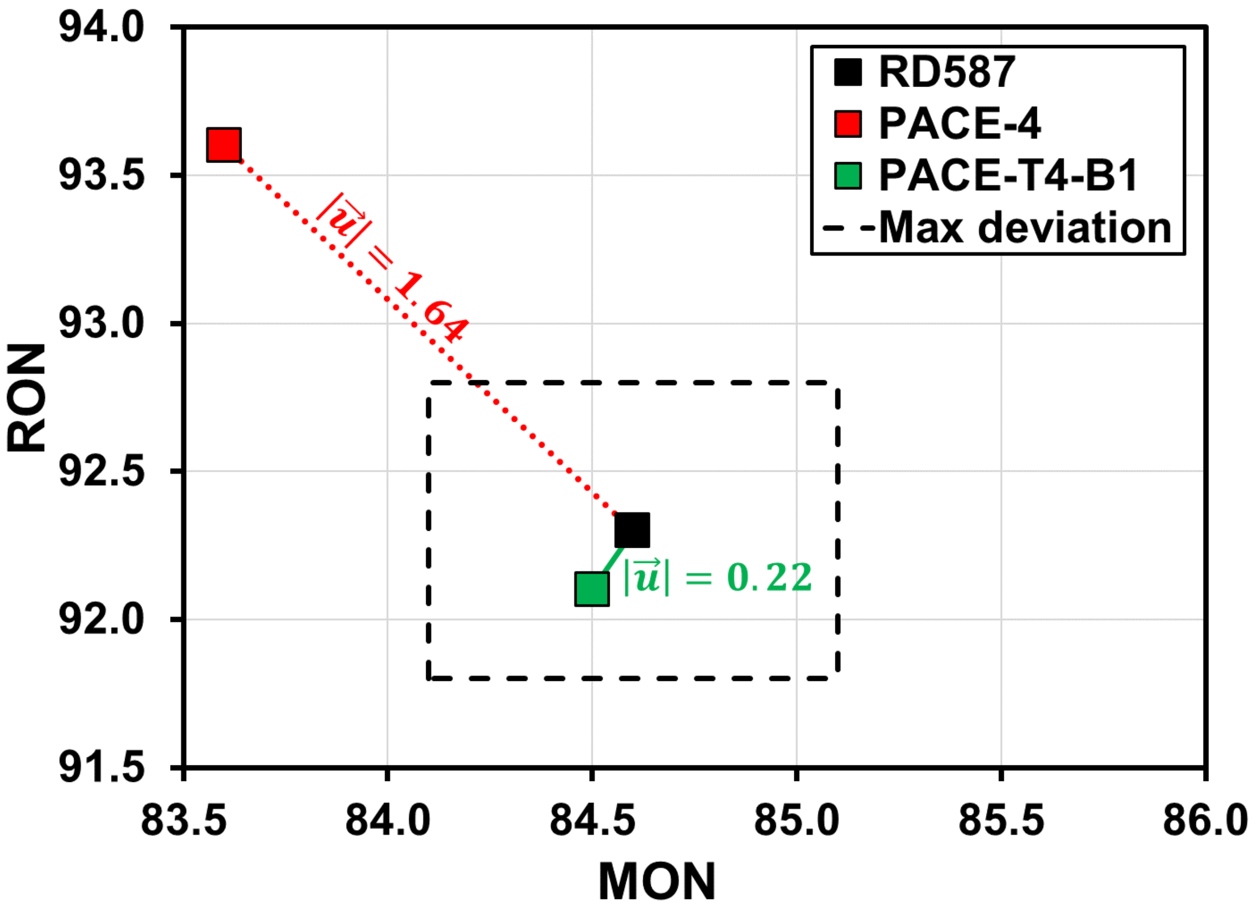
1. Quader, AA. "What limits lean operation in spark ignition engines—flame initiation or propagation?" SAE Paper 760760, 1976. doi:10.4271/760760

Matching the RON & MON of Surrogates with RD5-87

- PACE-4 predicted to match RON-MON within 0.32 units.
- However, measured RON-MON values were found to be 1.64 units from the values for RD5-87.



- For design of PACE-T4-B1 surrogate, compensate for the error in the RON-MON prediction by offsetting the target.
- Resulted in a very close match between measured RON-MON of the surrogate and that of RD587, 0.22 units.



Surrogate Fuel Design Procedure – Flow Chart